Atomic and Molecular Databases

« Open Science for better science and a sustainable world »

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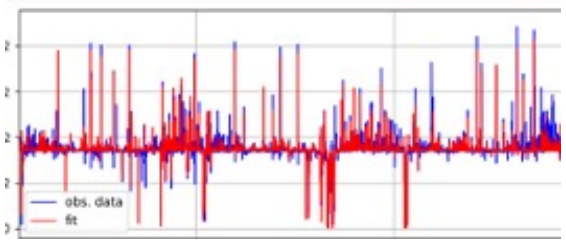
Disclaimer :
Any error in describing the material provided by my colleagues is only mine.
Any mistake in presenting material describing national, international institutions and governments activities is only mine.

Current Responsabilities : Chair of VAMDC consortium (up to Nov 2022), Vice-President of IAU B5 Commission,
Chair of B2-B5 WG on “Lab. Astro. Data”

Astro. Scientific Questions

Life Cycle of Astro Data

Astronomical Observations
mm, submm (ALMA, ..)
IR (JWST, ..)
UV (LUVOIR, ..)
Optical (ELT, VLTI, ..)
X (CHANDRA, ATHENA,..)



Astrophysical Spectra
(or images)

Standards : IVOA

Modelisation of the Objects
physical model of the object
atomic and molecular processes <-> A&M Data

Analysis of Observed Spectra : models object, radiative transfer methods
atomic and molecular processes <-> A&M Data

Life Cycle of A&M Data

Issues with atomic and molecular data
lack of existing data for many processes
improve accuracy of the A&M data

Lab. Astro Challenges

Trigger for new experiments
Trigger for new calculations

Data

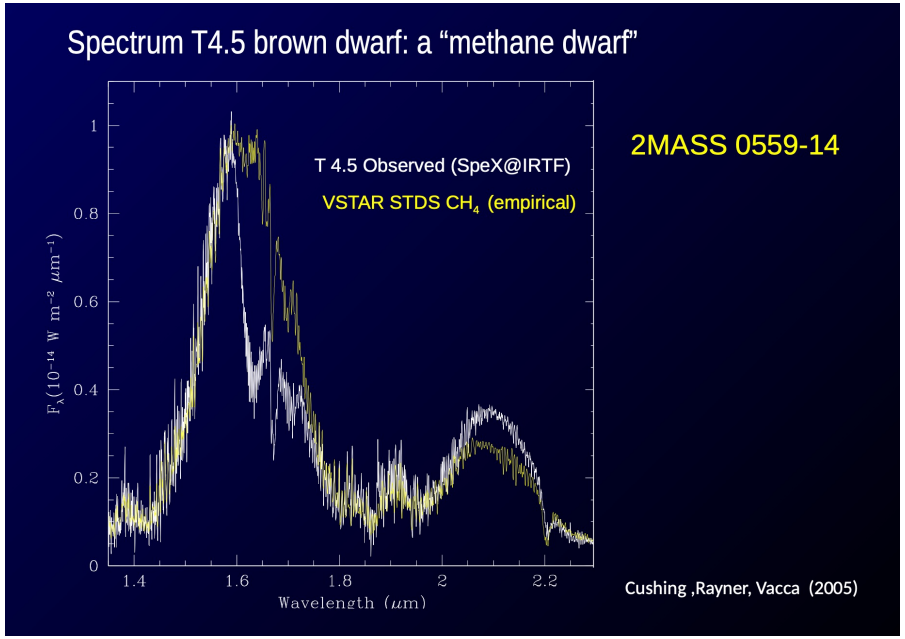
easy access to the A&M data
tracability of the A&M data
citation of the A&M data

Lab. Astro. Data

Databases
Distribution of A&M data
Good Practices with management of A&M data
Interfaces with astro tools and astro codes

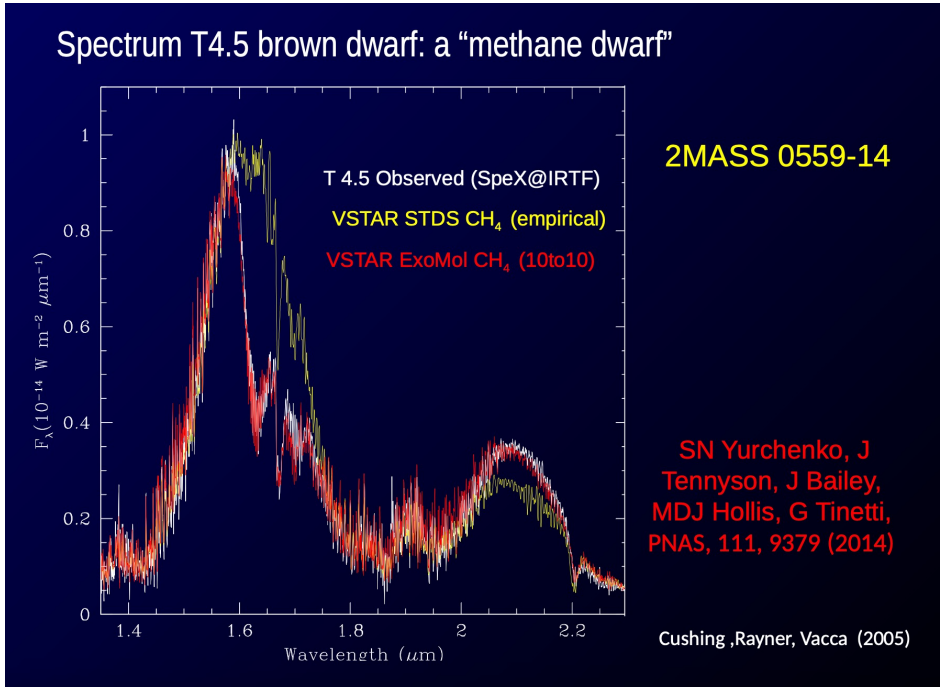
An example : How knowledge on astrophysical object Progresses thanks to new calculations

Courtesy of J. Tennyson, UCL, London, UK



9 years later
With the **ExoMol Data** On CH_4
(200 times more data than
Previously : High Temperature)

2005 →



ExoMol Molecular line lists for exoplanet and other atmospheres
Jonathan Tennyson and Sergey Yurchenko (UCL)

I. BeH, MgH, CaH
II. SiO
III. HCN/HNC
IV. CH_4
V. NaCl, KCl
VI.PN
VII. PH_3
VIII. H_2CO
IX. AlO
X. NaH
XI. HNO_3
XII. CS
XIII. CaO
XIV. SO_2
XV. HOOH
XVI. H_2S
XVII. SO_3
XVIII. VO
XIX. $H_2{}^{18}O$, $H_2{}^{17}O$
XX. H_3^+

Hot line lists; Published in MNRAS

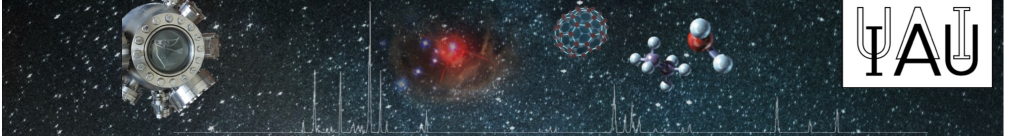
XXI. NO
XXII. SiH_4
XXIII. PO, PS
XXIV. SiH
XXV. SiS
XXVI. SN, SH
XXVII. AlH
XXVIII. C_2H_4
XXIX. CH_3Cl
XXX. $H_2{}^{16}O$
XXXI. C_2
XXXII. TiO
XXXIII. MgO
XXXIV. PH
XXXV. NH_3
XXXVI SH (UV)
XXXVII HCCH
XXXVIII SiO_2
XXXIX CO_2
XL. H_3O^+
XLI. NaOH, KaOH
XLII. NO (UV)
XLIII. NaO
XLIV. SiO (UV)
XLV. MgH, CaH (UV)

erc

Formal data releases:
J. Tennyson *et al.*, J. Mol. Spectrosc. **373**, 73 (2016)
and JQSRT **255**, 107228 (2020)

ExoMol database features
www.exomol.com

1. Line lists
2. Cross-sections
3. Partition functions
4. Broadening parameters
   (Barton et al, JQSRT **187**, 453 & 203, 490 (2017))
   H_2 and He: J and T dependence (only)
5. k-tables
6. Lifetimes (Tennyson et al, J Phys B, 49, 044002 (2016))
7. Cooling functions
8. Lande g-factors (Semenov et al, J Mol Spectrosc (2016))
9. Dipoles for molecular control/orientation effects
   A Yachmenev, RichMol project (Owens et al, Sci Rep 7, 45068 (2017))
10. Application program interface (API)
11. Opacity tables (in 4 formats) (Chubb et al. *A&A*, **646**, A21 (2021))
12. LiDa: Lifetimes database
13. ExoMolHR: high resolution spectra
14. New! Temperature dependent photodissociation cross sections



A) Needs from Astrophysics (and other fields)

- Possible list : species, processes, range [energies/temperature/frequencies/other parameters], precision
- The above list impacts Prioritization for experimental set ups and for calculations (systems, methodologies, ..)
- 그래서 “Everything” is not a criteria ! (”sic” from a recent paper ☺).
- “Better science and a sustainable world” : how ?
  - Share information (Open Science culture)
  - Collect and combine ”Needs” (per domain, instruments, ..)/Use White Papers
  - Keep trace of the “Needs” in an open and indexed repository (F.A.I.R.)
  - Make the process as self-sustainable as possible

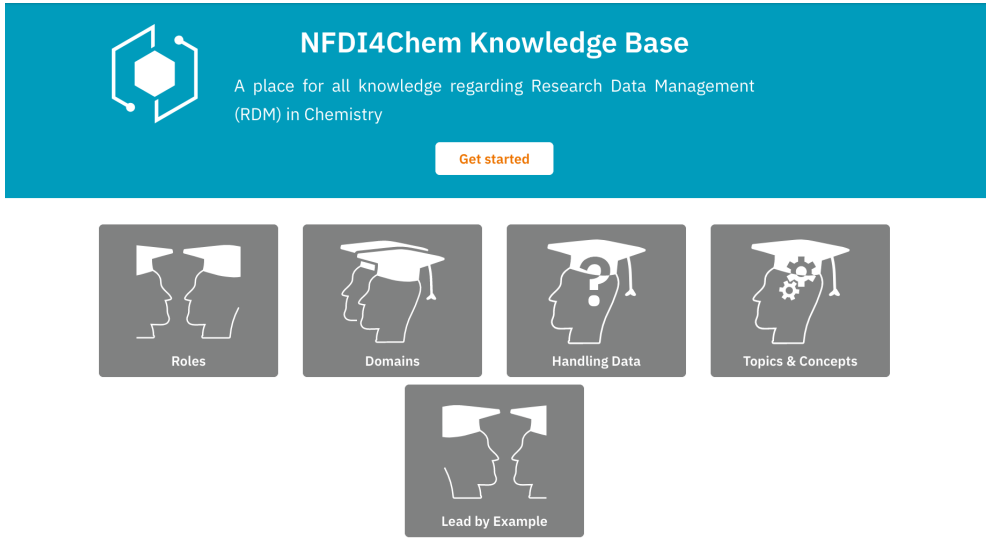
B) Fields of A&M&Solid Physics : Experimental & Theoretical Challenges

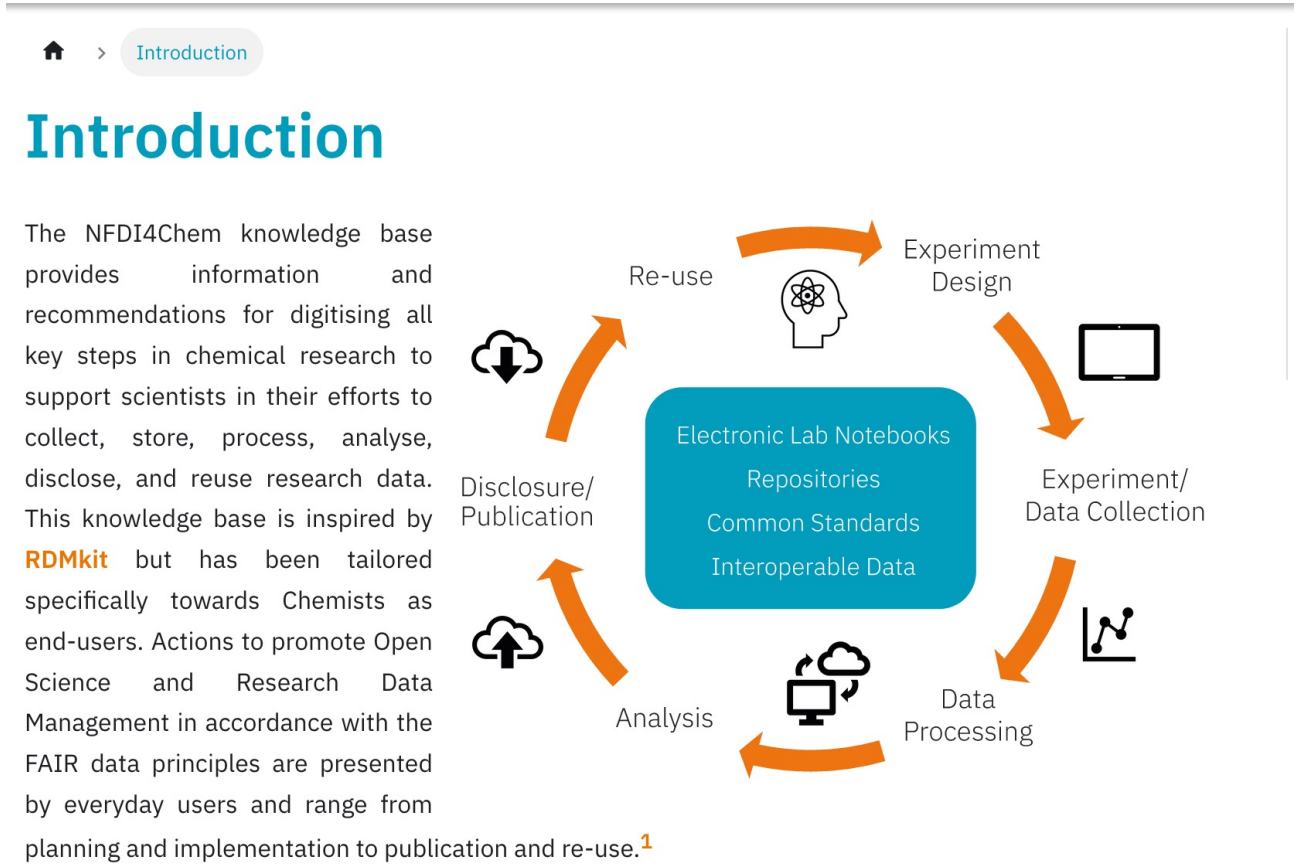
- Design and Decision - Projects
  - Projects are usually funded (Description of planned objectives, systems, methodologies, expected results). “80% is well described in the proposals”
  - Research Data Management Plan is also part of those funded projects
- Develop instrumentations, analysis software, numerical codes
- Obtain “Primary Data”
  - Store on repositories (Zenodo, University, National, International)
  - Possibly in Databases
- From “Primary Data” to “Secondary Data”
  - Internal or external post-treatment
  - Usually stored in “thematic” databases
  - “Needs in application fields” are usually those “Secondary Data”

Taking as an example this morning talk on collisional excitation of species by heavy particles (A. Faure)

- Primary data could be :
  - Potential Energy Surface Points and other ab initio quantities , obtained from a quantum chemistry code
  - Fitting code and parameters of the Potential Energy Data Points
  - Cross-sections or diffusion matrices as a function of collision energy obtained with a dynamical collision code
  - Can be re-used to obtain “secondary data” for astrophysics or re-used for other purposes by physicits and quantum chemists
- “Secondary Data” could be :
  - State-to-state rate coefficients as a function of temperature and as function of all internal states of of both target and collider
  - “Thermalized” state-to-state rate coefficients as a function of temperature and as function of the internal states of the target but averaged for the collider
  - **Latest are used by astrophysicts in non-LTE analysis of ISM & cometary atmospheres**

RDM – Need for support to communities
Example of Chemistry For Chemists as end-users
https://knowledgebase.nfdi4chem.de/knowledge_base/





Funded by DFG Deutsche Forschungsgemeinschaft German Research Foundation
NFDI4Chem is funded by DFG
Project Number 441958208

Examples of Repositories

(Often needed for Research Data Management Plans)

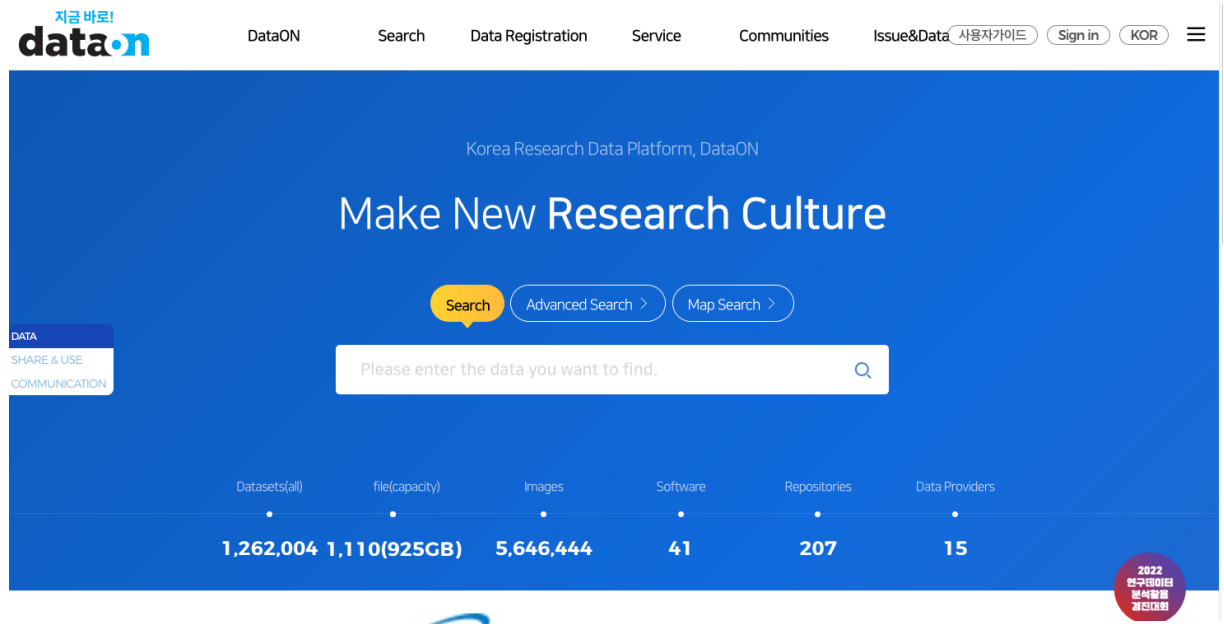
- ZENODO : https://zenodo.org/
- EUDAT : https://sp.eudat.eu/
- National Platforms

https://www.openaire.eu

Indexed in

Collect metadata

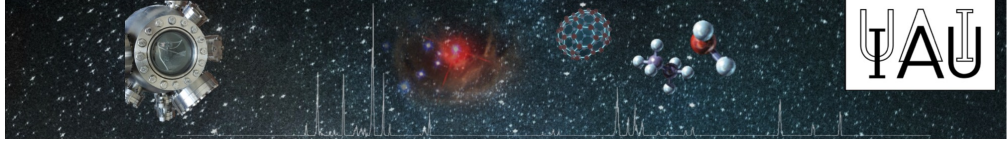
https://dataon.kisti.re.kr/



RÉPUBLIQUE FRANÇAISE
Liberté
Égalité
Fraternité
recherche.data.gouv.fr

An ecosystem for sharing and opening research data
FEDERATE, SUPPORT, SHARE, OPEN, REUSE

Actions to help communities to share their data
Interconnect different thematic repositories
Etc …



“A better science and sustainable world”

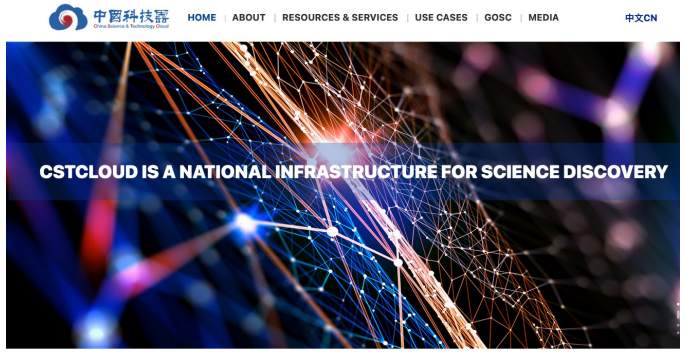
- Share information about activities of groups (yesterday morning B5 commission session) in an open, indexed and self-sustainable repository
- As projects are funded and well described
  - Share in an open, indexed and self-sustainable repository some information of the project (with as much sincerity as possible) : systems, methodology, approximate milestones
- Share and index the “primary data” on repositories that can be mined
  - Use standard indexing
- Include your secondary data in existing thematic databases (possibly in addition to supplementary material of journals). →. Part C
- Community should be continously informed on the available national and international platforms and on the various Open Science Initiatives

Open Science Clouds
Open Science Initiatives

UNESCO Recommendation on Open Science

The UNESCO Recommendation on Open Science was adopted by the General Conference of UNESCO at its 41st session, in November 2021.

- UNESCO Recommendation on Open Science
  English | Français



EUROPEAN OPEN SCIENCE CLOUD

About Services & Resources

EOSC Portal - A gateway to information and resources in EOSC

COMMITTEE ON DATA CODATA INTERNATIONAL SCIENCE COUNCIL

About M

Global Open Science Cloud

ARDC Australian Research Data Commons

ABOUT US SERVICES COLLABORATIONS

nfdi Nationale Forschungsdaten Infrastruktur

Open Science in Korea:"the OECD acknowledged the 2017/2018 Korean initiative on sharing and reuse of publicly funded research data with the objective to promote big data-driven innovation at national level"
https://community.oecd.org/docs/DOC-141310

Digital Research Alliance of Canada | Alliance de recherche numérique du Canada

nationaal programma open science

National Programme Open Science

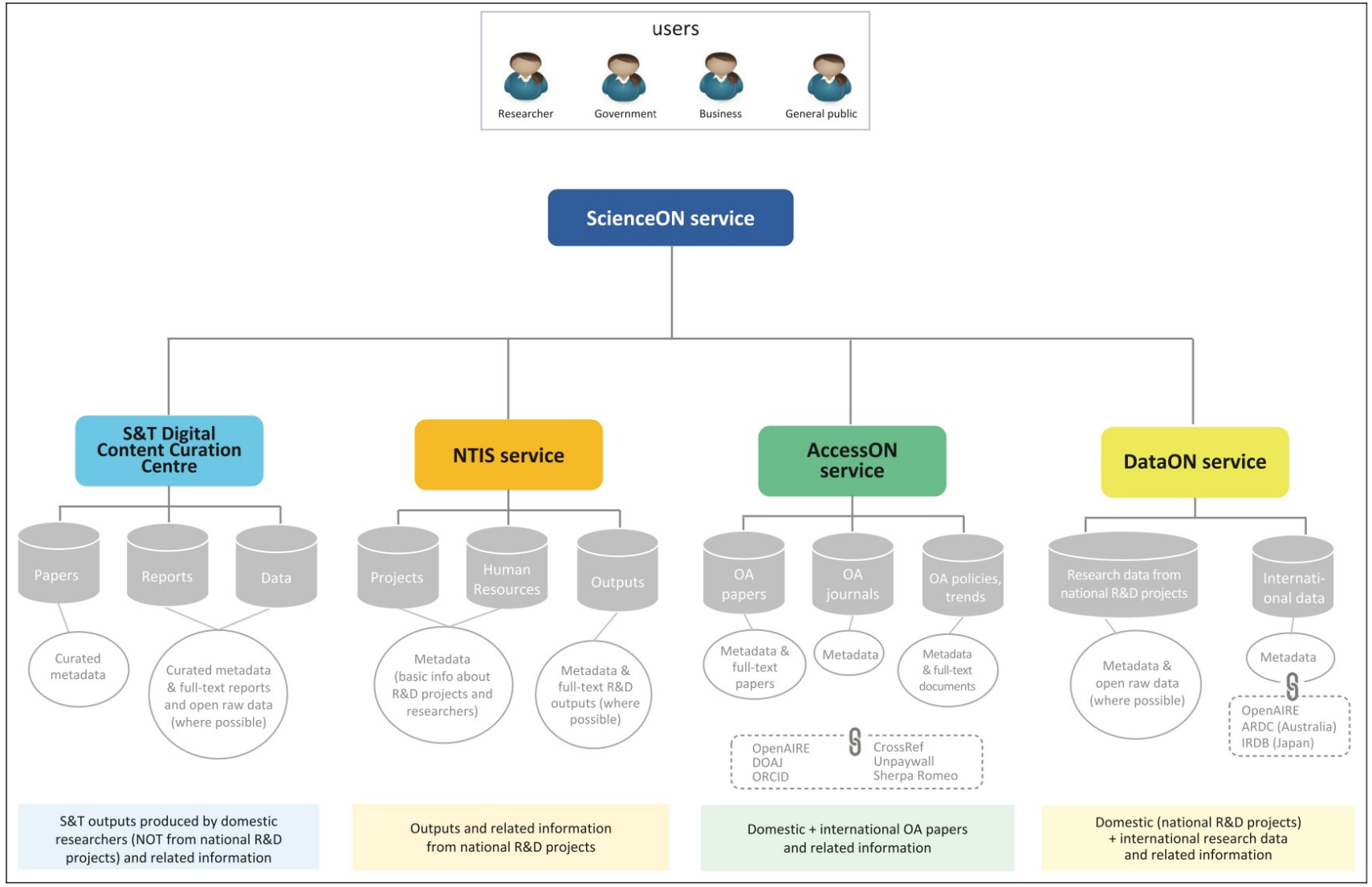
MINISTÈRE DE L'ENSEIGNEMENT SUPÉRIEUR ET DE LA RECHERCHE
Liberté Égalité Fraternité

Ouvrir la science ! OPEN SCIENCE

Malaysia Open Science Platform Focus Areas

1. National Guideline
2. National Policy
3. Management
   - Data Management Plan
   - Capacity and Capability of Data Management
   - Data Managers

Korea Institute of Science and Technology Information



igure 1. National Open Science digital infrastructure operated by the Korea Institute of Science and Technology Information (KISTI) and provided knowledge resources.

"Korea's national approach to Open Science: Present and possible future", H. Shmagun, J. Sim, K-N Choi, J. Kim
J. of Information Science, 1-20, 2022,
DOI:10.1177/01655515221107336

Second French Plan for Open Science – Launched 6 July 2021

MINISTÈRE DE L'ENSEIGNEMENT SUPÉRIEUR ET DE LA RECHERCHE

Path One : Generalising open access to publications

1. **Generalise the obligation to publish in open access** all articles and books resulting from publicly funded calls for proposals
2. **Support open access economic publishing models** that do not require the payment of articles or books processing charges ("diamond" model)
3. **Encourage multilingualism** and the circulation of scientific knowledge by translating publications by French researchers

"Our goal is to reach **100% of open access publications**"

" We will support **bibliodiversity** so that the scientific community can regain control over the publishing system."

MINISTÈRE DE L'ENSEIGNEMENT SUPÉRIEUR ET DE LA RECHERCHE

Path Two : Structuring, sharing and opening up research data

4. **Implement the obligation to disseminate publicly funded research data**
5. **Create Recherche Data Gouv**, an ecosystem for sharing and opening research data
6. **Promote widespread adoption of data policies** that cover the whole lifecycle of research data, to ensure that they are Findable, Accessible, Interoperable and Reusable (FAIR)

« We will encourage practices that favor **research data reuse.** »

« We will create Recherche Data Gouv in order to **involve all research fields in active practices of open data.** »

MINISTÈRE DE L'ENSEIGNEMENT SUPÉRIEUR ET DE LA RECHERCHE

Path Three : Opening up and promoting source code produced by research

7. **Recognize and support the dissemination under an open source license of software** produced by publicly funded research programmes
8. **Highlight the production of source code** from higher education, research and innovation
9. Define and promote an **open source software policy**

« The opening of software source code is a major challenge for the **reproductibility** of scientific results. »

« Distribution of software products under **open source licence** will be preferred. »

MINISTÈRE DE L'ENSEIGNEMENT SUPÉRIEUR ET DE LA RECHERCHE

Path Four : Transforming practices to make open science the default principle

10. **Develop and value open science skills** throughout the educational and career pathways of students and research staff
11. **Value open science and the diversity of scientific productions in the assessment** of researchers, of projects and of universities and research performing organizations
12. **Triple the budget for open science** through the National Fund for Open Science and the Investments for the Future Programme

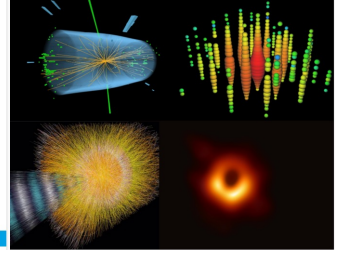
« Transformation of the assessment system is required in order to **foster long-term open science practices.** »

um, Ko

Particles, Universe, NuClei and Hadrons for the NFDI

A consortium in the NFDI.

PUNCH 4NFDI



GERMANY

https://www.punch4nfdi.de/

Germany

The prime goal of PUNCH4NFDI is the setup of a federated and "FAIR" science data platform, offering the infrastructures and interfaces necessary for the access to and use of data and computing resources of the involved communities and beyond. The High-Level Milestones of the PUNCH4NFDI consortium can be seen here: (PDF, 42KB)

nfdi4phys CONCEPTS ABOUT CONSORTIUM NEWS RESOURCES CONTACT

Nationale Forschungsdateninfrastruktur für disziplinäre und transdisziplinäre Physik

Use cases

Atoms and Molecules

- UC AtoMol1 Prof. Dr. Stephan Schlemmer, University of Cologne
- UC AtoMol2 Prof. Dr. Piet Schmidt & Dr. Fabian Wolf, National Metrology Institute (PTB), Braunschweig

Physics of Plasma

- UC Plasma01 Dr. Dirk Uhrlandt & Prof. Dr. Ronny Brandenburg & Dr. Markus Becker, Leibniz Institute for Plasma Science and Technology (INP), Greifswald
- UC Plasma02 Prof. Dr. Achim von Keudell & Dr. Marina Prenzel, Ruhr-University Bochum (RUB)
- UC Plasma03 Alexander Kessler, Helmholtz Institute Jena (HI Jena)

C) Data and Databases Challenges

C1. Preparation : Scientific Aspects

- Collection of data
- Cleaning/verification of data
- Sometimes evaluation of data
- Possibly aggregation of data : complete dataset A with dataset B
- Association of Information to the data such as methodologies, codes, etc..
- Association of References to the data (and their DOI)
- Association of metadata to the datasets
- Each database has an “input” or “ingestion” format
- Time consuming, highly specialized → change of culture for collecting data is necessary → templates filled by producers

C1. Ingestion : Data Model Aspects

Data Models of thematic Databases influence the template for the “input” file of the database

- Example of CollisionDB
- Example of SSHADE
- Example of BASECOL

Combined data of collisions and spectroscopy from different provenances : other DB and producers – **Output Format of RADEX code (User)**

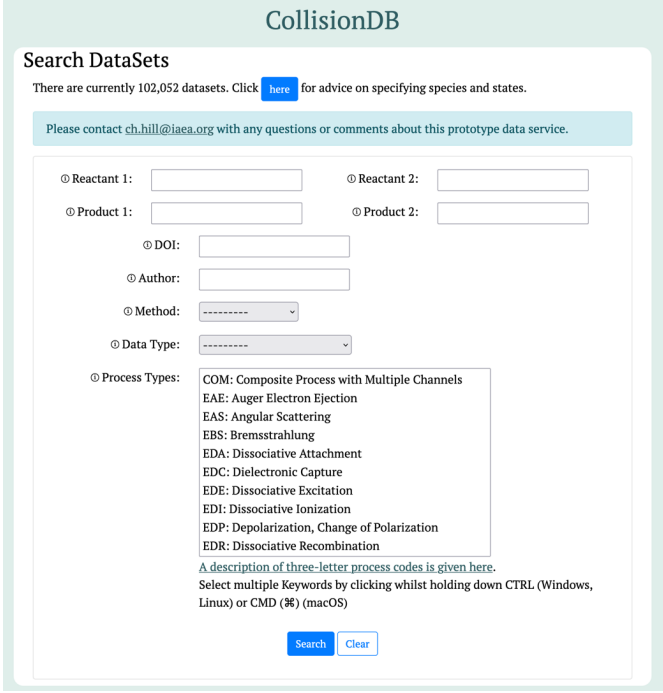
- services are Websites with stored flat files :
  - Example of LAMDA : https://home.strw.leidenuniv.nl/~moldata/
  - Example of CASSIS Database associated to the CASSIS analysis software http://cassis.irap.omp.eu/
- Similar service : EMAA : https://emaa.osug.fr/
  - Input format into relational DB
  - Output format in “RADEX” format

IAEA
International Atomic Energy Agency
Atoms for Peace and Development

Christian Hill, Dipti
Martin Haničinec
Atomic and Molecular Data Unit
Nuclear Data Section

CollisionDB

https://db-amdis.org/collisiondb



- **CollisionDB** is a database of plasma collisional processes (cross sections and rate coefficients)
- For nuclear fusion energy, astrophysics, and other research
- Searchable by “reactant”, “product”, DOI, author, process type

Data Ingestion

- Data providers may use a simplified, key-value pair format
- Uncertainties can be a fixed percentage or per-data point
- Standards for processes, species and states (**PyValem :** https://github.com/xnx/pyvalem)
- Standards for units (pyqn)
- Related processes can be combined into a single file

```
comment="Adiabatic-nuclei calculations performed with the spheroidal MCCC(210) moc
method="MCCC"
doi=["10.1006/adnd.1997.0736"]
data_type="cross section"
threshold="1.229E+01"
uncertainty="10%"
columns=["E, eV", "sigma, a0^2"]

reaction="e- + H2 X(1SIGMA+g); v=0 -> e- + H2 C(1PIu); v=0"
process_types=["EXE","EXV"]

E              sigma
1.229E+01   1.0129E-03
1.250E+01   1.089E-03:1.07E-05
1.267E+01   1.173E-03:2.44E-05
1.403E+01   1.551E-03
...
```

Courtesy of Christian Hill

Courtesy : B. Schmitt, Observatory of Grenoble, France

https://www.sshade.eu/ **SSHADE**

- **Provide to the planetary and astrophysics community**
  - **Spectral and spectro-photometric data**
    - on all types of solid materials (but also liquid)
    - from synthetic, terrestrial or extraterrestrial samples
  - **Bandlist data**
    - on fundamental minerals and simple molecular solids
  - **with well documented information !!**
    - on the spectra, samples, experiments … + publications
  - **with a data reference and a DOI per experiment**
    - easy to cite & provides direct access to the data used

➔For the analysis, modeling and interpretation of spectroscopic observations of planetary surfaces, small bodies, cosmomaterials, aerosols & grains, + inter- & circumstellar grains, exoplanets…

- **Materials**
  - **Ices** (low/high T-P, mixtures, …), molecular solids, snow…
  - **Minerals,** rocks
  - **Organic solids,** polymers, **Carbonaceous materials,** …
  - **Inorganic solids**, Metals, …
  - also some **liquids**

- **Samples**
  - **Synthesized** in the laboratory
  - **Natural terrestrial analogues** collected or measured in the field
  - **Cosmomaterials collected on Earth**: (micro-)meteorites, *IDPs,* …
  - **Extra-terrestrial samples** collected on planetary bodies: lunar soils…

Data Ingestion

- **Fill the sample xml file: describe the state, composition and other required metadata**
- *Option:* **give details about preparation protocol of your sample**
- **Validate the xml : Data / Import** (tick the box " ignore missing ressources")
- **If necessary Zip with image or documentation files**
- **Import the sample**
  - verify all data are OK using « Provider / Search / Sample » to search and visualize it
  - You can change anything by using "correction" in import mode.

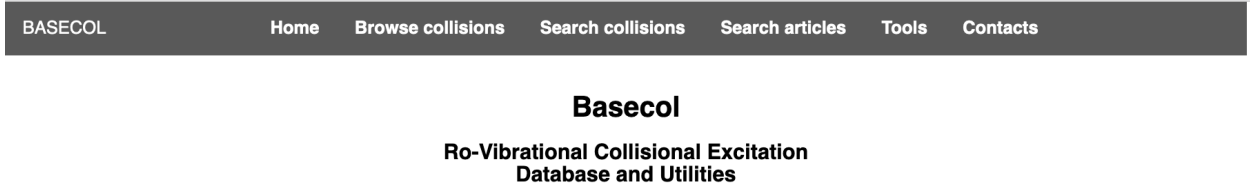
✓ Note: your sample xml file will be also stored 'as it is' in the DB and retrievable with the 'import history' tab

- **Spectral ranges:**
  - Designed from γ-rays to radio wavelengths
  - Now mostly **from VUV to sub-mm (0.2µm - 1mm),** plus **X-rays**.

- **Types of data:** (from level 1 to 5)

➢ **Spectra**
  - **Transmission** spectra, absorption coefficients,
  - **Optical constants** …
  - **Reflectance** spectra of surfaces, spectro-photometric functions, …
  - **Raman** spectra & micro-spectroscopy, *Fluorescence*, …
  - **XANES** spectra

Aim and Ingestion : BASECOL https://basecol.vamdc.eu/



- Provide to the astrophysics community (ISM, cometary) and Chemical-Physics community
  - State-to-state Inelastic Collisional Rate Coefficients allowing energy transfer in both the target and the collider
  - A visibility of different datasets for the same collisional systems : species and processes
  - A bibliography associated to the datasets
  - A description of methodologies with associated references
  - A versioning system allowing for minor and major updates : different versions being available to the user
  - **Metadata for VAMDC interoperability** and for BASECOL interface

BASECOL2020 New technical Design, Atoms 2020, 8, 69

A decade with VAMDC : Results and Ambitions, Atoms, 2020, 8, 76

Follow standards of VAMDC for description of Quantum Numbers : **XSAMS** standard for atoms and the **case-by-case now maintained at IAEA for the molecules** https://amdis.iaea.org/cbc/

Use InchI/InchIKey standards from IUPAC

```
## DIRECTORY : TARGET
## FILE : element_.dat
$$name = HCl
$$inchikey = VEXZGXHMUGYJMC-UHFFFAOYSA-N
$$inchi = InChI=1S/ClH/h1H
$$stoichiometricFormula = ClH
$$htmlName = HCl
$$latex = HCl
$$mass = 35.97
$$molecularConstant = 317504.5911
$$charge = 0
$$elementType =  molecule

## FILE : origin_.dat
$$case = dcs
$$symmetry = none
$$quantumNumbers = J
#   Level              Energy             J
       1                   0             0


## FILE : energy_.dat
$$case = dcs
$$symmetry = none
$$title = Rotational energy levels of HCl (used in Lique & Faure, 2017)
$$comments = The rotational energy levels are obtained from the H$_2$Cl PES (Bien et al. 2000) using a DVR method.
$$type = theoretical
$$quantumNumbers = J

#  Level                  Energy             J
       1           0.0             0
       2          20.9             1
       3          62.5             2
       4         125.0             3
       5         211.2             4
```

TARGET SECTION

SPECIES

ENERGY

C2. Access to the Data

- Via DB Website and Downloads of Files
- Via FTP request
- Via computer access using own developed software tools
- Via an e-infrastructure

The NASA Ames PAH IR Spectroscopic Database (PAHdb)

https://www.nasa.gov/ames/spacescience-and-astrobiology/the-nasa-ames-pah-ir-spectroscopic-database-pahdb)

Presentation at IAU GA 2022, Division B, 8th August by Christiaan Boersma

Documentation Portal
NASA Ames PAH IR Spectroscopic Database

Welcome to the NASA Ames PAH IR Spectroscopic Database Documentation Portal. More information about the NASA Ames PAH IR Spectroscopic Database (PAHdb) can be found at the PAHdb website. Below you can access the website documentation, documentation describing the different software Application Programming Interfaces (APIs) and a cookbook with recipes for using the (software) tools.

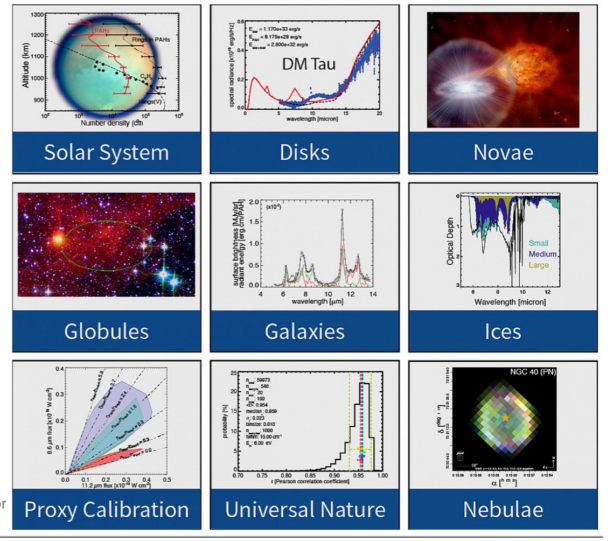
Website Manual

website

AmesPAHdbIDLSuite (repository) | *AmesPAHdbPythonSuite* (repository) | *pyPAHdb* (repository)

Cookbook

The NASA Ames PAH IR Spectroscopic Database is being supported through a directed Work Package at NASA Ames titled: "Laboratory Astrophysics – The NASA Ames PAH IR Spectroscopic Database".



Astrochem-tools (https://astrochem-tools.org/)

Services developed and maintained at the Observatoire Aquitain des Sciences de l'Univers (OASU) and the Laboratoire d'astrophysique de Bordeaux (LAB) for the astrochemical community.

KIDA — **KInetic Database for Astrochemistry**
http://kida.astrochem-tools.org/

ISA — **InterStellar Abundance database**
http://isa.astrochem-tools.org/

ACN — **AstroChemical Newsletter**
http://acn.astrochem-tools.org/

Nautilus — **Nautilus gas-grain code**
https://forge.oasu.u-bordeaux.fr/LAB/astrochem-tools/pnautilus

Astrochemical Forum — **Astrochemical forum**
https://discourse.astrochem-tools.org/

Courtesy of Coordinators: Pierre Gratier and Valentine Wakelam

KIDA KINETIC DATABASE FOR ASTROCHEMISTRY

Funding

Cosmic PAH portal

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http://cosmic-pah.irap.omp.eu

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COSMIC PAH portal

Description

Polycyclic aromatic hydrocarbons (PAHs) and related molecular species (e.g. fullerenes) are key species in astrophysical environments. The primary objective of the Cosmic PAH portal is to ease access to databases and tools in order to:

- **Identify** these species in astrophysical environments and in extraterrestrial samples.
- **Understand** their formation pathways and their link with related molecular species such as carbon clusters and fullerenes.
- **Model** their evolution in astrophysical environments and their impact on the physical and chemical conditions.

Link content

- **Molecular databases** developed by the team, both theoretical and experimental.
- **Simulated spectra databases** for PAH infrared emission in various astrophysical environments.
- **Spectral analysis tools** to analyze in a consistent way spectra from experiments. theoretical calculations, and astrophysical observations.
- **Tools to model spectra** in astrophysical environments using experimental and theoretical data.

AtomDB http://www.atomdb.org/

Purpose:

The AtomDB project is a combination of a database of atomic data and the plasma models required to convert these into spectra useful for analysing astrophysical X-ray spectra.

The Database (APED):

Species of interest: Thermal X-ray emitting astrophysical spectra are largely He- and H-like ions of elements up to Nickel and L-shell emission from Fe and Ni. AtomDB has data for all ions of all elements up to Nickel, though the above are more well checked.

Data Types: Centered on modeling optically thin, collisionally ionized plasmas. Therefore there are energy levels, bound-bound wavelengths and transition probabilities, electron and proton excitation collision strengths, electron impact ionization and recombination, dielectronic satellite lines etc etc.

Data Sources: Data is largely from published theoretical calculation, with experimental benchmarks where available. Data is stored as FITS files and publicly available for download. Data which needs interpretation – e.g. extracting rate coefficients from fitting formulae – have publicly available python packages to aid extraction.

The Models/Codes (APEC):

Thermal Plasma: Most commonly used model, collisional ionized plasma emissivities for equilibrium and non-equilibrium plasma.

Charge Exchange: Modeling charge transfer from, e.g. neutral H to solar wind ions.

Non-Maxwellian Plasma: Modeling plasma with a 'kappa' electron energy distribution.

Courtesy : Adam Foster, CFA, Harvard, USA

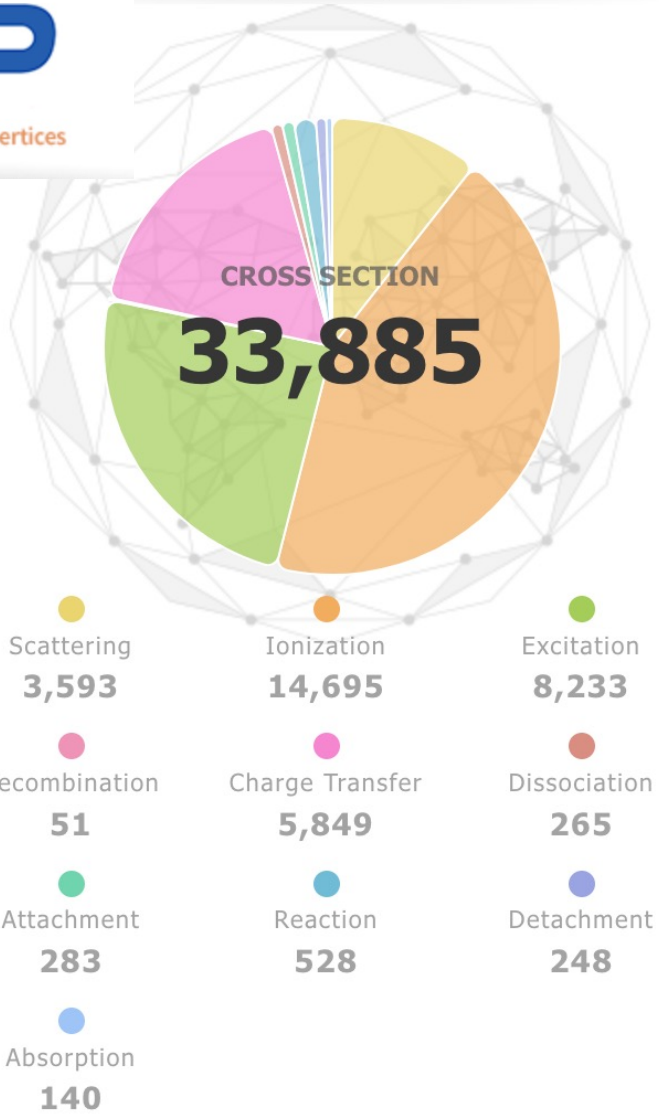
Korean Databases For Plasmas

KFE KOREA INSTITUTE OF FUSION ENERGY

https://dcpp.kfe.re.kr/index.do

Collision

DCPP Data Center for Plasma Propertices



KAERI Korea Atomic Energy Research Institute

https://pearl.kaeri.re.kr/pearl/

Photonic Electronic Atomic Reaction Laboratory

Atomic Data Center in KAERI

Access the Atomic Databases

Database on Photoionization/Electron Impact Ionization/Dielectronic Recombination Cross Sections and Rate Coefficient

Go ➜

Database on CR-Model for Helium

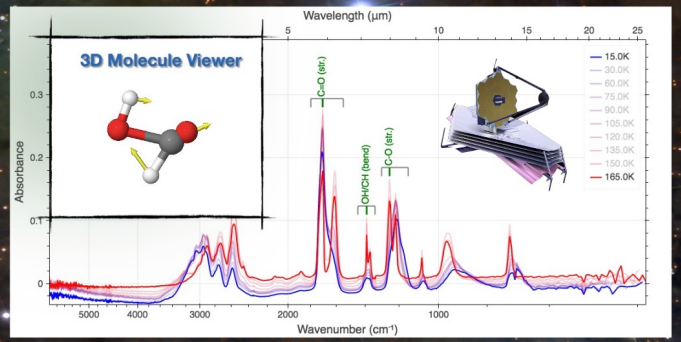
Electron Impact Excitation Rate Coefficient

Go ➜

LIDA [Leiden Ice Database for Astrochemistry]
icedb.strw.leidenuniv.nl

Next Talk by W. Rocha

Example:
IR spectrum:
HCOOH:



JWST/ERS
ICE AGE

Sent by
H. Linnartz

1068 different spectra; different compositions; different mixing ratios; range of astrophysically relevant temperatures; analytical tools, for assignments and spectral simulations
Designed to fully support JWST ice observations

Next Talks given

- On the LIDA Database
- On the NIST-LANL Lanthanide Opacity Database

National Institute of Standards and Technology
U.S. Department of Commerce

Los Alamos NATIONAL LABORATORY

PML Website | About This Database

NIST-LANL Lanthanide Opacity Database

Karen Olsen[1], Christopher J. Fontes[2], C.L. Fryer[2], A.L. Hungerford[2], R.T. Wollaeger[2], O. Korobkin[2], Yuri Ralchenko[1]

Element / Nuclear Charge
La 57
Ce 58
Pr 59
Nd 60

Mass density ρ (g/cm^3) 10^{-4}

Electron Temperature (eV) 1

Photon energy (eV)
(between 1.25×10^{-5} eV and 1.5×10^{5} eV) .1 - 1

Opacity (cm^2/g)
(please select one opacity type for multiple element selection)
- all
- total opacity
- scattering opacity
- absorption opacity
  - bound-bound
  - bound-free
  - free-free

Submit

This work was supported by NASA (Grant 80HQTR19T0051) through the National Institute of Standards and Technology and by the U.S. Department of Energy through the Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001).

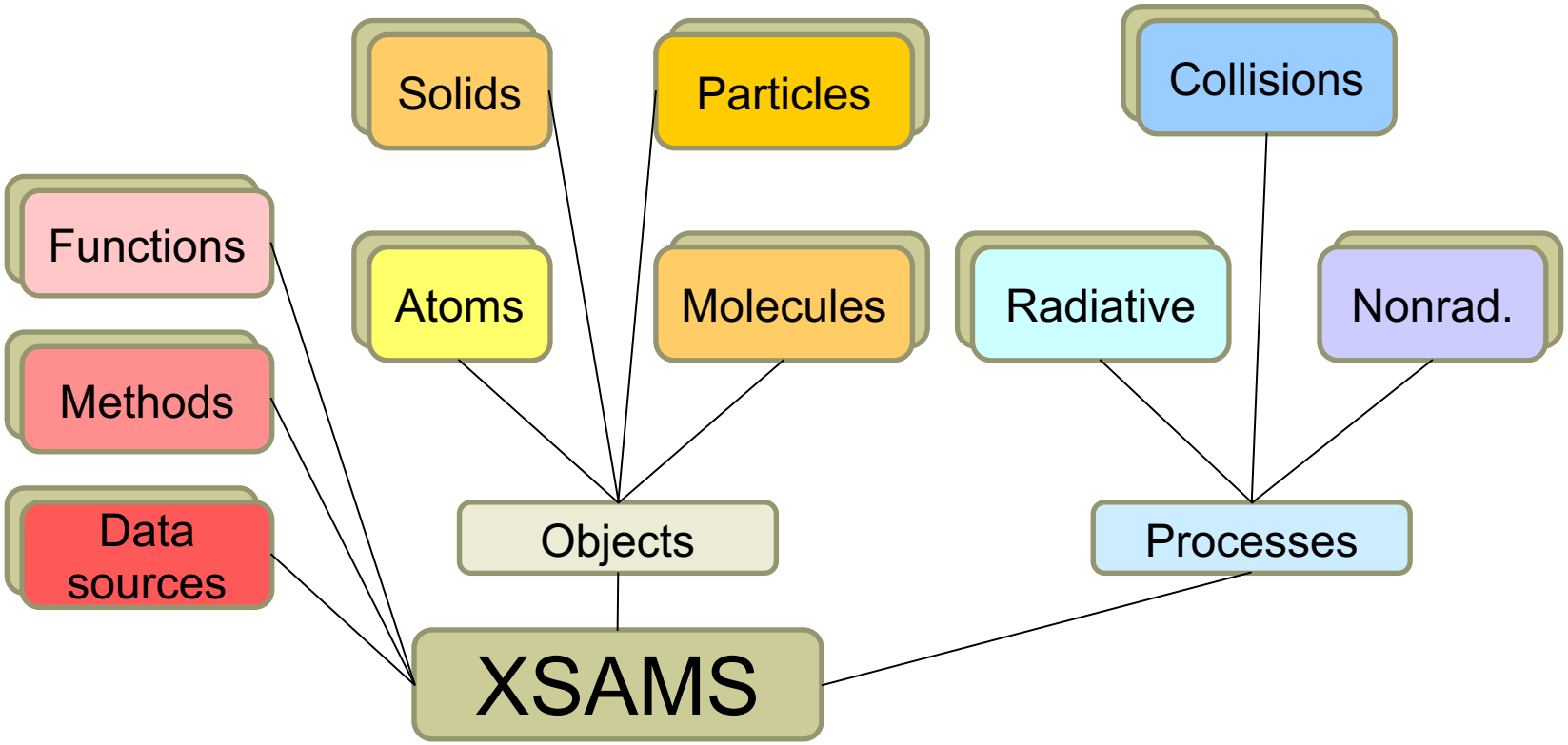
[1]National Institute of Standards and Technology, Gaithersburg, MD 20899

C3. Standards (input and/or output)

- HITRAN or CDMS (their own internal and output format very well known in the atmospheric and astrophysics communities -→ became “standards”)
  - http://hitran.org ; https://cdms.astro.uni-koeln.de/classic/entries/
- SSDM : Data Model and schema for SSHADE DB
- VAMDC Standards (Queries,Vocabularies,Registries, Dictionnaries) and in particular XSAMS Standard (NIST, IAEA, VAMDC)

Data Description : XSAMS format

XSAMS tree: XML Schema for Atoms, Molecules and Solids



(Courtesy Yuri Ralchenko)

Y. Ralchenko

R.E.H. Clark,
D. Humbert
B. Braams

D.R. Schultz, ORNL; E. Roueff, ML Dubernet, N. Moreau : Observatoire Paris; S. Gagarin, P.A. Loboda, VNIITF

D) E-science Infrastructures → Community oriented

SSHADE : : Provided by B. Schmitt, Obs. of Grenoble, France

VESPA : Provided by S. Erard, Obs. of Paris, France

VAMDC : an e-science platform for the exchange of Atomic and Molecular Data (vamdc.org)

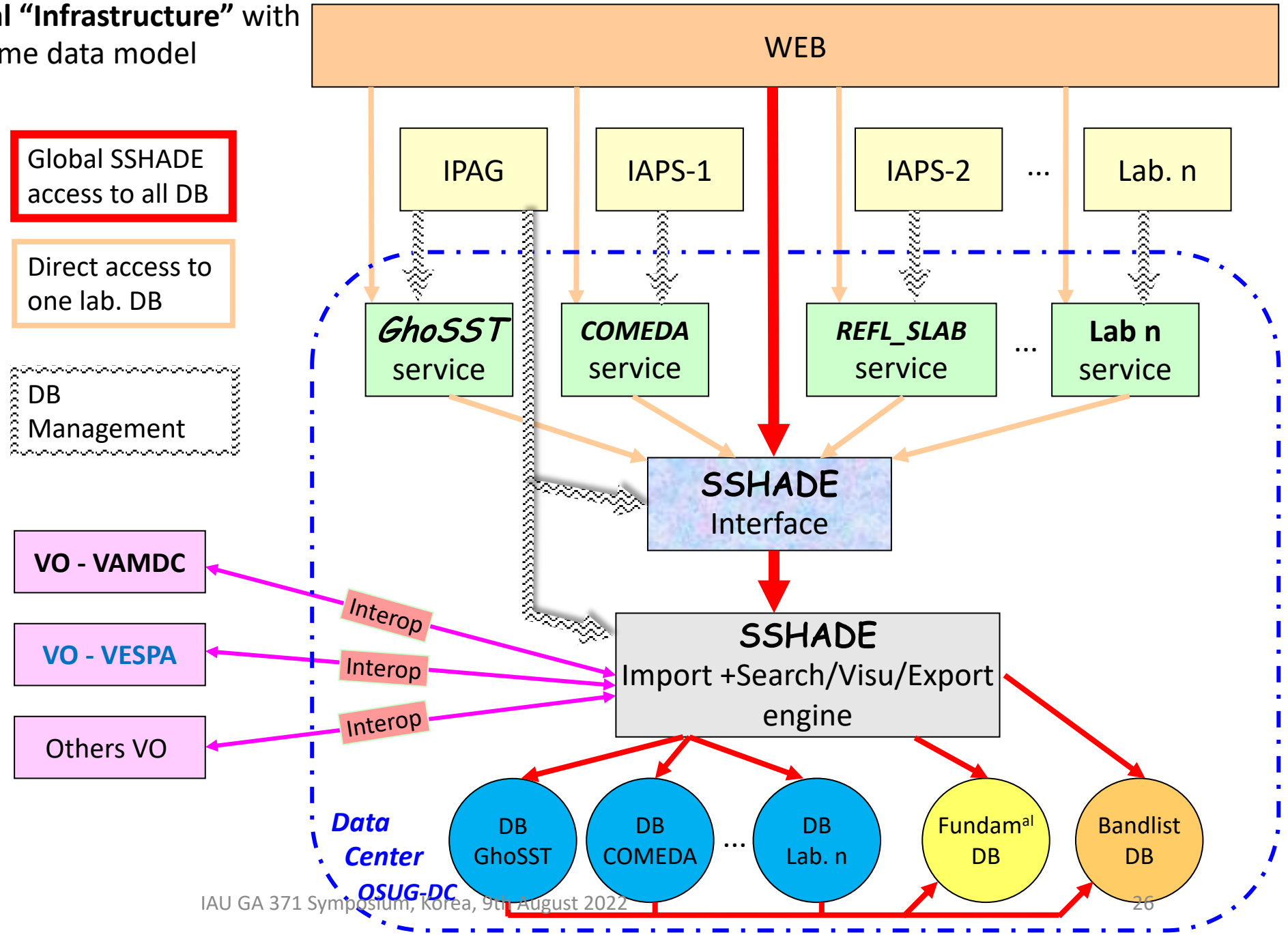
SSHADE : both a DB and a local "Infrastructure" with many small "DB" following same data model

Made of:

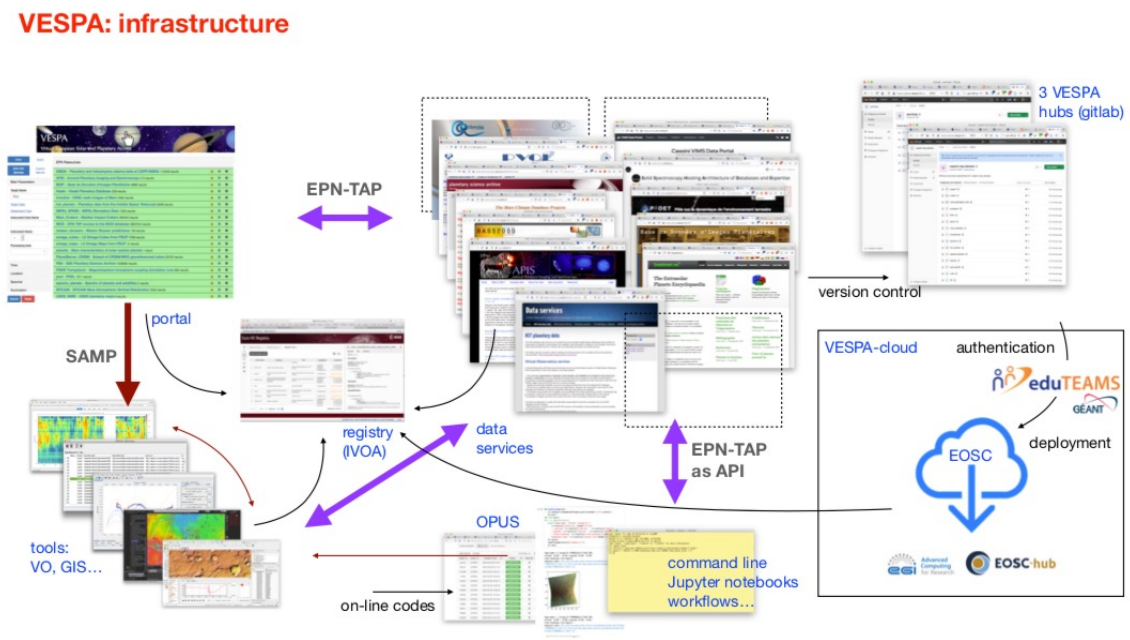
- ✓ A 'solid spectroscopy' interface
- ✓ A Search / Visualization / Export engine
- ✓ A set of databases:

  one per group
- ✓ A common fundamental database

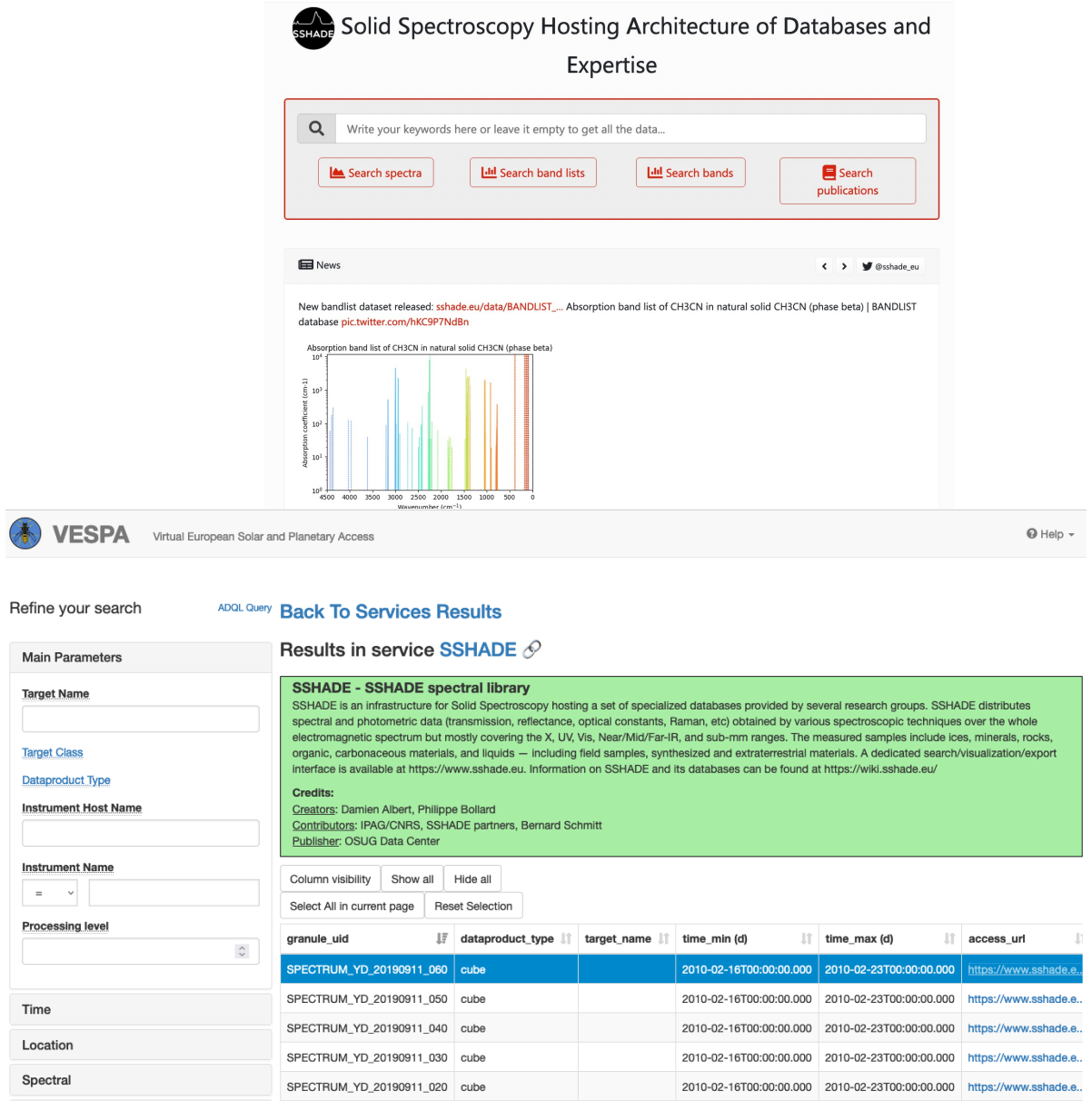
- Hosted at OSUG data center
- service of others VO



VESPA from EuroPlanet : imbedding SSHADE

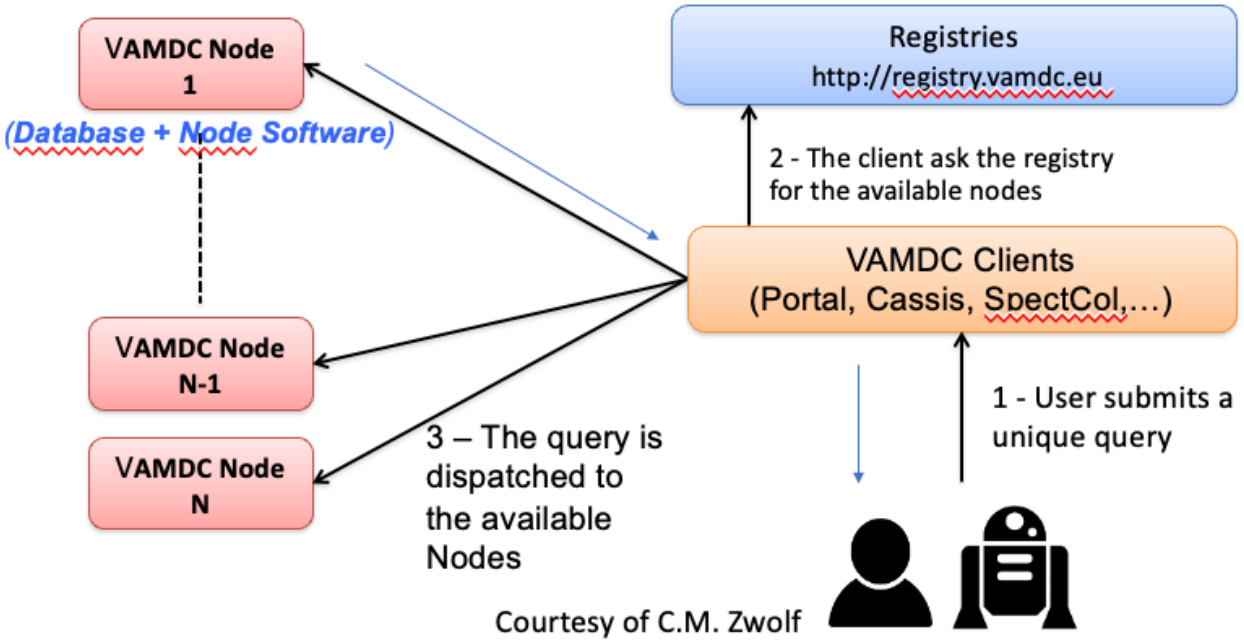


Access : give URL pointing to datafiles



The Virtual Atomic and Molecular Data Centre
http://www.vamdc.org

VAMDC
Interoperable access to 37 heterogeneous A+M Databases



- E-infrastructure connecting about 37 heterogenous databases that can be accessed from http://portal.vamdc.org/
  Or any VAMDC compatible tools
- And a Consortium of partners sustaining their nodes and the core components of the infrastructure
- High quality scientific data come from different Physical/Chemical Communities

Paper « A decade with VAMDC : results and ambition, Atoms, 2020 »
http://dx.doi.org/10.3390/atoms8040076

Databases	Type of A&M Data	Partners	Application's Fields
NIFS AMDIS IONIZATION	Electron-impact ionization cross-sections and rate coefficients (atoms & atomic ions)	National Institute for Fusion Science, Toki, Japan, I. Murakami	Stellar, Solar, plasma, fusion
VALD	Atomic Linelists	Uppsalla, Vienna, Moscow – N. Piskunov	Stellar -Solar
NIST Atomic Spectra	Spectroscopy of Atoms –	NIST – Yuri Ralchenko	Stellar – ISM -
CHIANTI	Atomic Linelists and collisions	Cambridge (UK)+MSSL/UCL – H. Mason, G. Rixon	Solar Physics
Spectr-W3	Atomic Linelists and Collisions	Russia (RFNC VNIITF) – P. Loboda	Solar/Stellar Physics + Fusion, plasma
Stark-B	Atomic LineShifts/Broadening with charged perturbers	Observatory of Belgrade (Serbia) + Observatory of Paris (LERMA) – M. Dimitrijevic/S. Sahal-Bréchot	Stellar Physics + Plasmas
TipBase, TopBase	Atomic Linelists and Collisions from Opacity Project and IRON Project	Observatory of Paris (LERMA) + CDS (Strasbourg, Fce) – F. Delahaye/C. Zeippen/C. Mendoza	Stellar, Solar Physics,
SESAM	Electronic Spectra of atoms and molecules	Paris Obs. – E. Roueff	ISM - Stellar

MOLD	Photo-Dissociation Cross-sections	Institute of Physics, Astronomical Obs, Belgrade, Serbia- Vladimir Sreckovic, V. Vujcic, D. Jevremovic	Stellar
BEAM-DB	Molecular/atom—electron collisions	Institute of Physics, Belgrade, Serbia Bratislav Marinkovi\'c	plasma, radiation damage
IDEABD	Dissociative electron attachment upon interaction of low energy electrons with molecules.	Innsbrück F. Duensing	Planets, ExoPlanets, ISM, Radiation Damage
AMBDAS	Collisions in plasmas (bibliographic) - searchable via processes ans species	IAEA, Vienna, Austria - C. Hill	Nuclear Fusion

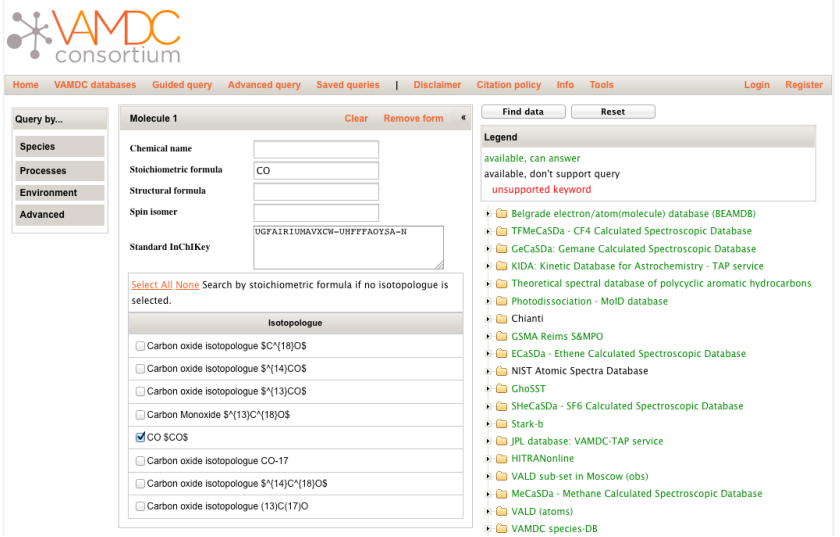
Databases	Type of A&M Data	Partners	Application's Fields
CDMS	Molecular Linelists (mm, Sub-mm)	Cologne (Germany) – S. Schlemmer	ISM + Earth+ CO
JPL	Molecular Linelists (mm, Sub-mm)	Pasadena (USA) + Cologne (Germany) – B. Drouin	ISM + Earth+CO
HITRAN	Molecular Linelists and Broadening Coefficients	Harvard (USA) + UCL – I. Gordon + L. Rothman	Earth, Planets, Exo-Planets
S&MPO	O_3 linelists	Reims (France)+ Tomsk (Russia) – V. Tyuterev	Earth – Exo-Planets
MeCaSDa	Linelists CH_4	Dijon (France) – V. Boudon	Earth, Planets, Exo-Planets, Brown dwarfs
SHeCaSDa	Sulfur Hexafluoride Calculated LInelists	Dijon – V. Boudon	Earth
TFMeCaSDa	Tetrafluoro-Methane calculated linelists	Dijon – V. Boudon	Earth
ECaSDa	Ethene Calculated LInelists	Reims – L. Daumont	Earth and Planets
GeCaSDa	GeH_4 Linelists	Dijon – V. Boudon	Planets
RuCaSDa	RuO_4 Linelists	Dijon – V. Boudon	Nuclear Industry
TFSiCaSDa	SiF_4 Linelists	Dijon – V. Boudon	Earth
UHeCaSDa	UF_6 Linelists	Dijon – V. Boudon	Nuclear Industry
CDSD-296	CO_2 Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets, Brown Dwarfs
CDSD-1000	CO_2 Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets, Brown Dwarfs
CDSD-4000	CO_2 Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets, Brown Dwarfs
NOSD-1000	N_2O Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets
NDSD-1000	NO_2 Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets
ASD-1000	C_2H_2 Linelists (intensity cut-off)	IAO, Tomsk – V. Perevalov	Earth, Planets

VAMDC CONNECTED DATABASES

Databases	Type of A&M Data	Partners	Application's Fields
PAH	PAH Theoretical Data and soon experimental Data	Observatory of Cagliari (Italy) – IRAP (Toulouse, France) – G. Mulas+C. Joblin	ISM, Planets, Earth
KIDA	Kinetic Data	Bordeaux (France) – P. Gratier & V. Wakelam	ISM - Planets
UdfA	Kinetic Data (ex-UMIST)	Belfast (UK) – T. Millar	ISM - Planets
BASECOL	Low Energy Molecular Collisions	Observatory of Paris – M.L. Dubernet	ISM - CO
LASP	Solid Spectroscopy Data	Obs. of Catania – G. Leto	Planets, ISM
GhoSST	Solid Spectroscopy Data	Grenoble (France) – B. Schmitt	Planets, ISM
W@DIS	Water Information System	IAO, Tomsk – A. Fazliev	Earth and Planets

To be connected to
VAMDC e-infrastructure : PEARL DB (KAERI, Korea), DCCP (KFE, Korea), ExoMolOP (UCL, UK), additional NIFS DB (Japan)

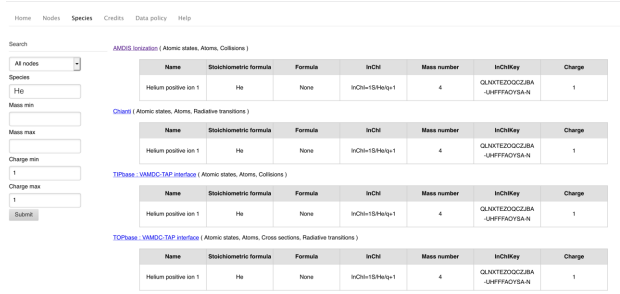
VAMDC Tools



Portal : Find, **A**ccess an retrieve **I**nteroperable resources across databases, to be **R**e-used, https://portal.vamdc.org/

Species Database : Interoperability on species ID

http://species.vamdc.eu (Inchi/InchiKey)



SPECTCOL : Take advantage of **I**nteroperability of Quantum Numbers

→ cross-match spectro (CDMS, JPL) & collisional data BASECOL) with Output in User Customized format with References & Unique Identifier (RADEX format)

Query Store : Reproductibility and Tracability → Assign Unique Identifier on queries and DOI through Zenodo

Technical Support : N. Moreau, Y.A. Ba, C.M. Zwölf

E) Re-use in Astrophysics Software Tools & Codes (A&M embedded)

IRAM Suite and YaFITS (Grenoble & Obs Paris, provided by J. Pety and P. Salomé)

XCLASS (Cologne, Provided by P. Schilke)

CASSIS (Toulouse, re-organised information from materials from J.M. Glorian)

Others - snapshots

Distributed Quick-Look Viewer for IRAM Archive


J.Pety, V. De Souza, S. Bardeau, E. Reynier, IRAM



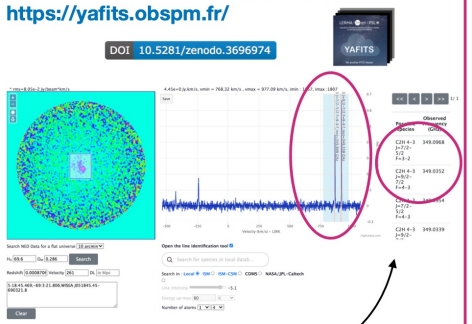

N. Moreau, Y-A Ba, M. Caillat, P. Salomé, LERMA, Observatoire de Paris

YAFITS@IRAM : Access and visualize IRAM archive (Large Programs) from the web **Quick-Look viewer inside the web-browser**

—> Planned for Early Spring 2022

Using YAFITS : a **distributed Quick-Look** FITS Viewer with **Line identification Tools**

https://yafits.obspm.fr/



VAMDC consortium **JPL / CDMS databases**

January 2021

Line catalogue access in IRAM software



J.Pety, S. Bardeau, E. Reynier, IRAM

IPAG Institut de Planétologie et d'Astrophysique de Grenoble

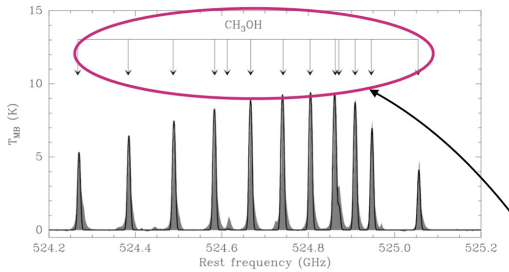
S. Maret, P. Hily-Blant, IPAG

WEEDS

An extension of the IRAM/CLASS software. It allows for **searches in atomic and molecular lines databases** (e.g. JPL or CDMS) via a **VO-protocol** **Maret, S. et al. , (2011)**

GILDAS SOFTWARE

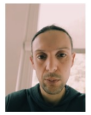
https://www.iram.fr/IRAMFR/GILDAS/




```
LAS> help weeds\

    Weeds is a CLASS extension to analyze spectral surveys or spectral lines
    observations with large bandwidths.  It  provides  several  commands  to
    identify lines on a spectrum and to model it.

    Available commands:
        LID      Identify lines on the current spectra
        LFIND    Find lines from a species within a frequency range
        LLIST    List lines from the line index
        LGET     Get a line from the line index
        LPLOT    Plot a line from the current line index
        MODSOURCE Model the emission of a source assuming LTE
        MODSHOW   Show the results of MODSOURCE

    For more information of each command, type 'help <command>'
LAS>
```

January 2021

ALMA Data Mining and Line identification



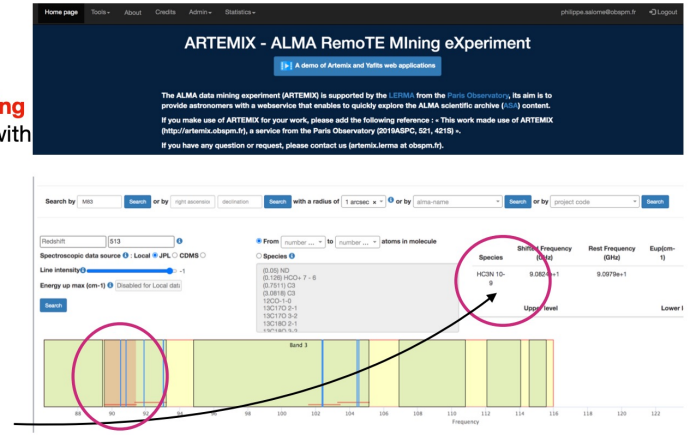

N. Moreau, Y-A Ba, M. Caillat, P. Salomé, LERMA, Observatoire de Paris

ARTEMIX : a **service to search and display** ALMA data (on-line since 2018).

An experiment for **data mining** the ALMA science Archive, with Line search tools. Also uses **Yafits**

http://artemix.obspm.fr/

VAMDC consortium **JPL / CDMS databases**



January 2021

NOEMA, French Alpes
12 15m antennas

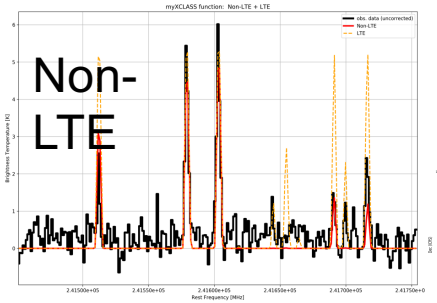
XCLASS Software

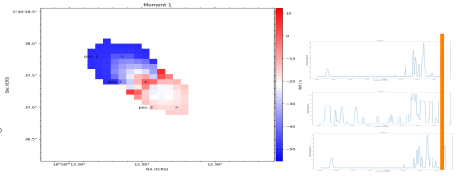
(P. Schilke and coll, Cologne University, Germany)

Automatic optimized fitting using radiative transfer

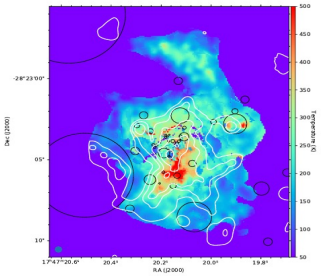
https://xclass.astro.uni-koeln.de

Data from VAMDC/CDMS

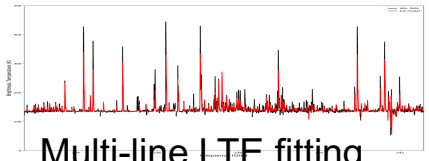




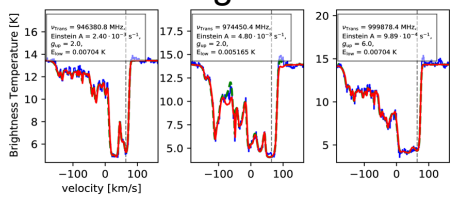
Physical model fitting



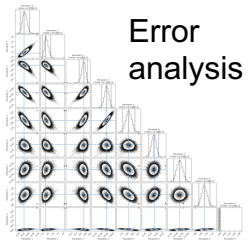
Physical parameter fitting in maps



Multi-line LTE fitting



Complex line shape fitting



Error analysis

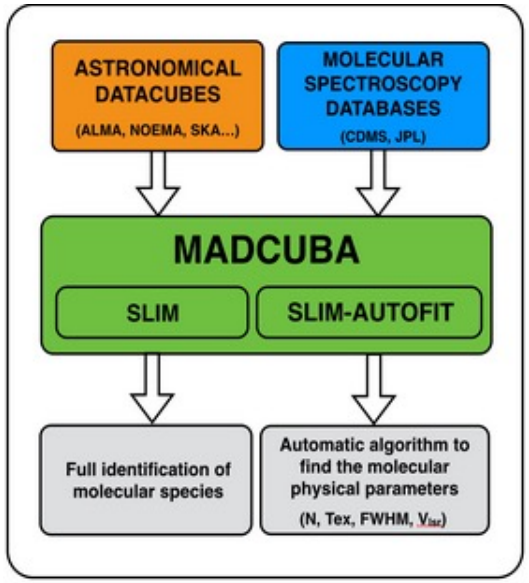
CASSIS Software :

http://cassis.irap.omp.eu

- Standalone Software that analyzes and models observations from ground or space-based observatories (mm, sub-mm for now).
- Has implemented VAMDC Queries to spectroscopic data (JPL, HITRAN, CDMS, NIST, etc ..)
- Contact : Charlotte Vastel and Jean-Michel Glorian (Toulouse University, Frce) - Jean-Michel.Glorian@irap.omp.eu, cvastel@irap.omp.eu

MADCUBA

https://cab.inta-csic.es/madcuba/



Analyse astronomical line data from both 3D spectroscopic cubes and single-pointing spectra

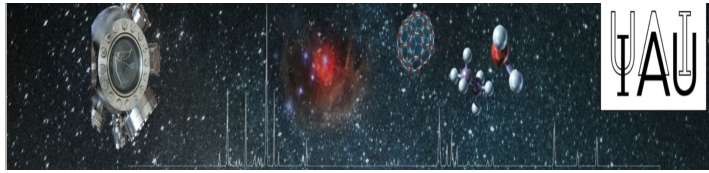
Some other tools (yesterday Talks at B5)

- ENIIGMA (https://eniigma-fitting-tool.readthedocs.io/) : ENIIGMA is a fitting tool to decompose the infrared spectrum of protostars containing ice features by using a linear combination of infrared laboratory data of molecules in the solid phase (Will Rocha)
- The NASA Ames PAH IR Spectroscopic Database Suite of tools : Laboratory-measured and quantum-chemically-computed IR spectra, models and tools for analyzing and interpreting the astronomical PAH signature (Christiaan Boersman)

A few examples of codes embedding A&M Data

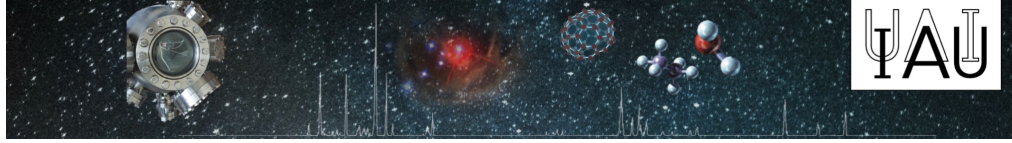
- ATOMDB : www.atomdb.org - Modeling spectra of collisionally ionized astrophysical plasma, focusing on X-ray astronomy (Adam Foster)
- CLOUDY : https://pa.as.uky.edu/gary/cloudy-project - Spectral synthesis code (ISM, exoplanets, astrophysical plasmas, ..) “Cloudy is a code that does this - it calculates the ionization, chemistry, radiation transport, and dynamics simultaneously and self consistently, building from a foundation of atomic and molecular processes. The result is a prediction of the conditions in the material and its observed spectrum.” (Gary Ferlan)
- MARCS : Code for 1D LTE model atmosphere production - https://marcs.astro.uu.se/ (bengt.edvardsson@physics.uu.se) → VALD DB
- PHOENIX : 1D+3D atmosphere modeling of astrophysical objects (exomplanets, all typs of stars, novae, supernovae) - https://ascl.net/1010.056 (Peter H. Hauschildt)

F) F.A.I.R. Issues



→ FAIR principles ensure Tracability of A&M&Solid Data that is an essential component to reproduce the analysis of observed data and the modelisation of the astrophysical objects

- **F**indable : Unique & persistant identifier for data and metadata, rich metadata, registration of metadata and data
- **A**ccessible : standardised, open, free communication protocols to retrieve data/metadata & metadata still available when data no longer available
- **I**nteroperable : data/metadata use a formal, accessible, shared and broadly applicable language for knowledge representation, FAIR vocabularies
- **R**e-usable : data/metadata richly described with accurate & relevant attributes, associated with detailed provenance, meet domain-relevant community standards



B5 IAU commission & Inter-Commission B2-B5 WG

- Commission B5 is a cross-disciplinary commission to promote “Laboratory Astrophysics”, i.e. Laboratory Data for Astrophysics
  - With WGs that to deliver reports about new science performed in the laboratories on molecular/atomic physics and now on data
- The B5 Commission was created to encompass the 4 fundamental research areas :
  - atomic and molecular astrophysics
  - dust and ices
  - plasma astrophysics
  - nuclear and particle astrophysics

WG “Laboratory Astrophysics Data Compilation, Validation and Standardisation: from the Laboratory to **FAIR** Usage in the Astronomical Community”

Started Dec. 2021 for 3 years

Outcome : Recommendations related to optimizing the process from laboratory data to astrophysics and vice-versa, taking into account **FAIR** principles

Most welcome to participate to the WG

Conclusions

- The first criteria of quality : the scientific expertise of the scientists who collect data and maintain databases → there is an issue about scientific sustainability → Change of Culture/Mentality : producers should fill « templates »

- The global context of data management, publication, access, re-use is getting more and more complex. Every country is pushing towards virtual environments and funders push towards being FAIR compliant. But Being FAIR compliant is NOT a simple issue. This relies on competent manpower available to develop and to sustain the resources/services → Make use of existing services

Conclusions

Finally InterPlay between Astrophysicists (Observers, Modelers) and Chemical-Physicists/Physicists (experimentalists and theoreticians) is essential to optimize science and resources and so, to participate to a sustainable world

- Publication of Needs in Astrophysics → *On-line Market Place updated with white papers and individual initiatives ?*
- Publication of Objectives of A&M&Solid Projects
- List of Resources : Groups/Activities, Databases, Services, Codes, Infrastructures (standards and services)
- Have WGs able to make recommendations (such as the B5 commission)

Long term Goal ?
“A better science and sustainable world”

Global Network of A&M&Solid Data for Astrophysics (and connected to other application fields as well ?)

- Part I : Build an Information system on lab. Groups, projects, needs, etc ..
  - Support/Extend the http://astrochemistry.eu initiative (*Dr Fuchs, Kassel Univ.*)

- Part II : Build a General indexing of resources (metadata)
  - To start an Interest Group at Research Data Alliance (https://www.rd-alliance.org/) in order to define the specifications
  → Brainstorming